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**Surface Relaxation Contributions to Axial Screw Dislocation Contrast in Synchrotron White-Beam X-Ray Topographs of SiC**

W. M. Vetter, M. Dudley (SUNY, Stony Brook)

Beamline(s): X19C

**Introduction**: The most characteristic defect in silicon carbide crystals is axial screw dislocations with Burgers vectors that are multiples of the c-lattice constant, called "micropipes" because they have hollow dislocation cores with diameters of 0.1 to 10 μm. Because the Burgers vectors of the superscrew dislocations are exceptionally large, aspects of defect contrast in x-ray topographs that are normally subtle in the images of dislocations of elementary dislocations (dislocations of normal strength), become pronounced. Images of axial superscrew dislocations arising from the distortion of lattice planes in directions normal to **b** by surface relaxation are described here, analyzed, and computer simulated using equations resulting from the elasticity theory of dislocations.

**Methods and Materials**: Topographs were obtained by allowing the highly collimated, area-filling beam of synchrotron white x-rays obtained from Beamline X19-C to fall onto thinned, basal-cut SiC wafers. The area-filling diffracted beams were recorded on 8 x 10" sheets of Kodak Industrex SR-5 film held normal to the incident beam direction either 10 cm behind (in the transmission geometry) or 10 cm before (in the back-reflection geometry) the crystal. For section topography, the synchrotron beam was restricted with a 50 μm slit. Computer simulations were carried out on a Pentium IV 2.0 GHz microcomputer. The code was written in C++. Generating an image of 200 x 200 pixels took 12 hrs of processing time. The results of a calculation were written to a data file and later plotted as a gray scale map with Microcal Origin 5.0.

**Results**: Micropipe images appeared in synchrotron white-beam x-ray topographs of thin, basal-cut SiC wafers taken using prismatic reflections where $\mathbf{g} \cdot \mathbf{b} = 0$. They consisted of white ovals inclined along the direction of the topographs' g-vector that were terminated with dark spikes at either end. The thin wafers tended to curl; the appearance of a defect's image varied depending on the sign of the curvature relative to the side serving as the diffracted beam's exit surface. The micropipe images were computer simulated using the ray-tracing method. The calculation assumed that they arose from the surface relaxation strain component of a closed-core screw dislocation perpendicular to the surface of a thin foil. The qualitative features of the micropipe images were reproduced in their simulations, but the magnitude of the lattice misorientations predicted by the model was not large enough to account for the size of the experimentally observed dislocation images. The qualitative resemblance between, for example, Fig. 1(a) and (b) confirmed that the x-ray topographic images of axial screw dislocations in prismatic reflections arise from surface relaxation strain. Taking into consideration sample curvature added greater lattice misorientation to the model, yet the size of the computed micropipe images remained about $^2\!/_5$ shorter along their long dimensions than the experimental topographs. Perhaps the surface of the hollow core permits further surface relaxation, resulting in the higher magnitude of orientation contrast than that predicted by the computer simulations. The elasticity equation upon which the simulation was based, did not take into account the presence of a micropipe's hollow core.

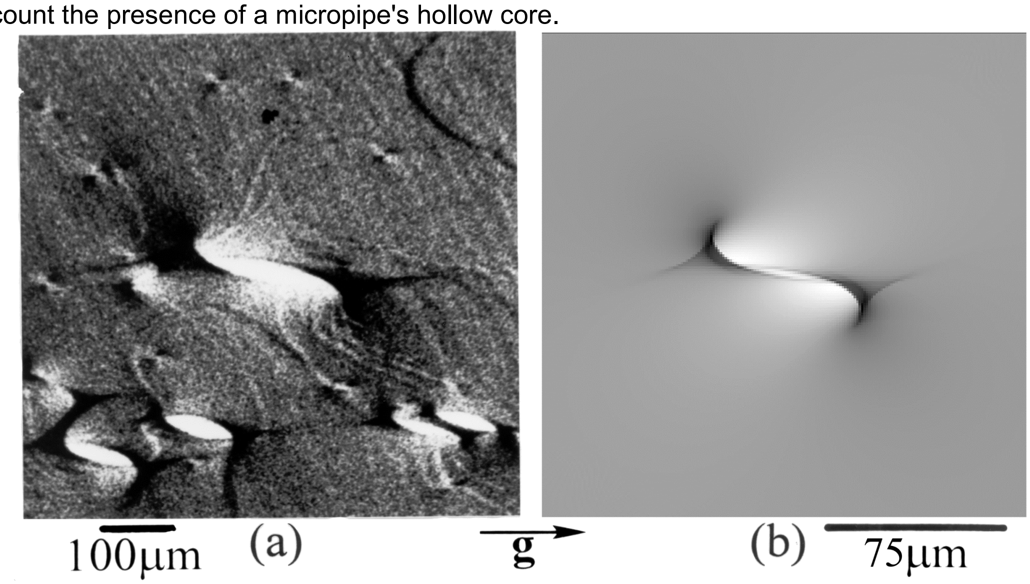


**Figure 1**. Transmission x-ray topograph of a 9**c** micropipe in a 15 μm thick SiC wafer: (a) actual (**g** = $11\bar{2}0$, λ = 0.59 Å) and (b) computer simulated.